N-(4-Bromophenyl)urea 967-25-5 | DTXSID3017333

1967-25-5	DTXSID301733

Model Performance

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Model	I)ata
Widdei	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 122 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.69e-01

Confidence level: 7.75e-01

Nearest Neighbors from the Training Set

Image not found

N-(4-Bromophenyl)urea

Measured: 115 Predicted: 122

Image not found

3-Bromophenylurea

Measured: 132 Predicted: 114

Image not found

(3-Methyl-4-bromophenyl)urea

Measured: 234 Predicted: 137

Image not found

3-Chlorophenylurea Measured: 102 Predicted: 57.3 Image not found

N-(3-chlorophenyl)-N'-

methylurea
Measured: 85.1
Predicted: 101